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MODELING THE PARAMETERS OF THE ELECTRONIC ATOMIC SHELL

Results of modeling parameters of the electron shell of atom such as orbital radius, constant of shielding and size of atom are presented in article. Based on the application of regression analysis, a complete scheme of the dependence of orbital radius on the charge number of the nucleus is constructed. Within the conducted research the dependence of the constant of shielding on ordinal value of the subshell of atom is revealed. The concept of the symmetric quantum number is offered. The possibility of semi-empirical estimation of the average size of atom with closed electron subshell is shown. Results of calculations are in satisfactory agreement with calculation and empirical data.

Keywords: atom, electronic subshell, orbital radius, nuclear charge, constant of shielding, quantum number.

[1-4].

[2].

[3].

[5]

[6]

[7]

$$K_r \sim \frac{Z - S}{a_0} \quad (1)$$

$$\Delta = \frac{3}{2} \frac{K_r}{l(l+1)} \quad (2)$$

/-

(1)

 K_r S

[8],

$$Z = f(a_d/r),$$

$$Z = (\quad) + 5, \quad (3)$$

 K_r S n

(3),

$$Y = Ax + B,$$

 A B K_r S

(1)

1.

1 -

-		K_r		S		
		(2)				%
1	15 ²	1,5	1,00	0,3	0,178	0,24
2	2s ²	1,5	1,56	2,05	0,67	0,07
3	2p ⁶	1,25	1,00	4,15	3,49	0,13
4	3s ²	1,5	1,57	9,15	5,68	0,11
5	3p ⁶	1,39	1,41	11,25	8,40	0,05
6	3 [^]	1,17	1,00	21,15	13,70	0,22
7	4s ²	1,5	1,50	25,65	17,65	0,04
8	4p ⁶	1,44	1,48	27,75	19,85	0,04
9	4J ¹⁰	1,31	1,21	39,15	27,60	0,18
10		1,13	1,17	50,55	30,46	0,06
11	5s ²	1,5	1,38	43,65	32,11	0,06
12	5p ⁶	1,46	1,43	45,75	41,93	0,08
13	~5cF ^o	1,38	1,17	71,15	53,95	0,08
14	5	1,26	1,39	62,55	57,05	0,10
15	6s ²	1,5	1,13	75,65	60,67	0,04
16	6p ⁶	1,47	1,03	77,75	67,77	0,16
17	6C ¹⁰	1,42	1,00	79,15	73,99	0,03
18	7s ²	1,5	1,18	84,8	73,02	0,04

K_r , $4/-$, $1,13$, $1,5$, $1^{\wedge}-$, $2^{\wedge}-$, $[3]$, $(S = 0,188)$ [5], $2^{\wedge}-$, $(S = 0,67)$, S , $(\dots 2)$, S , $0,24 \%$.

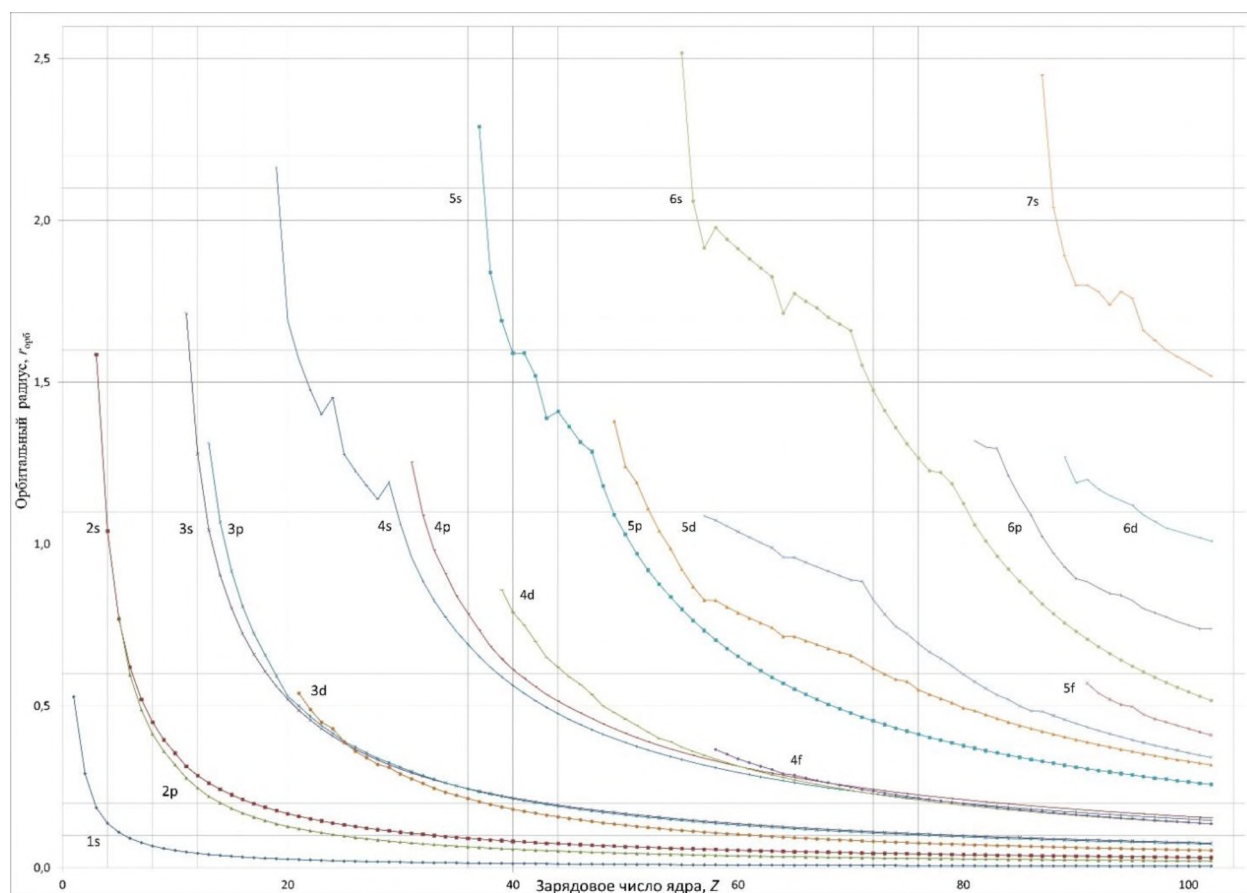


Рисунок 1 – Схема изменения орбитальных радиусов r_{orb} (в ангстремах)

Z

1

 Z .

«

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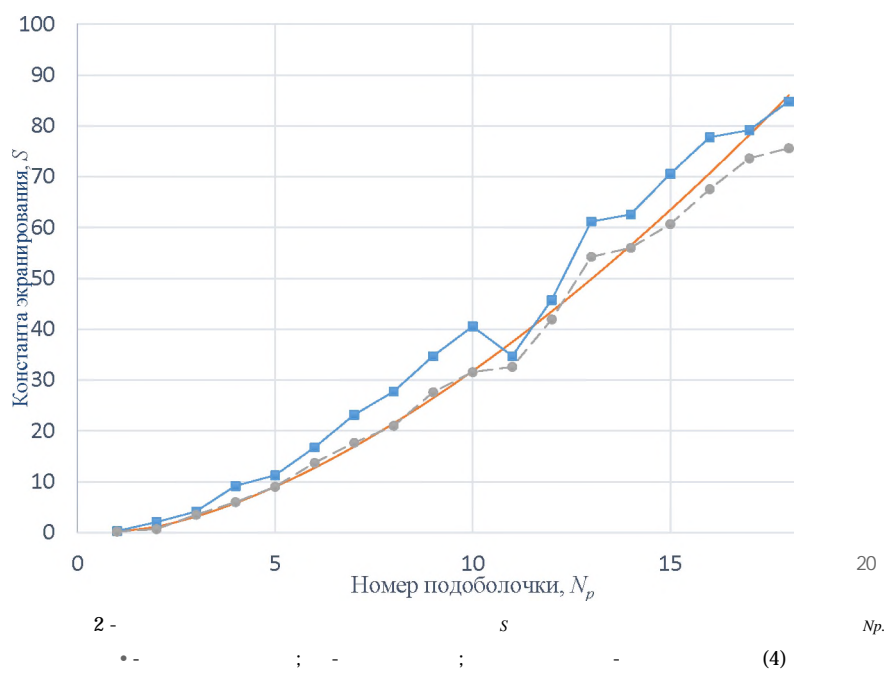
»,

[8],

,

,

,

($Z = 60$), N_p .

2

 S S

$$S = (N_p - 23)^{1/2}. \quad (4)$$

 N_p , K

3,

 K

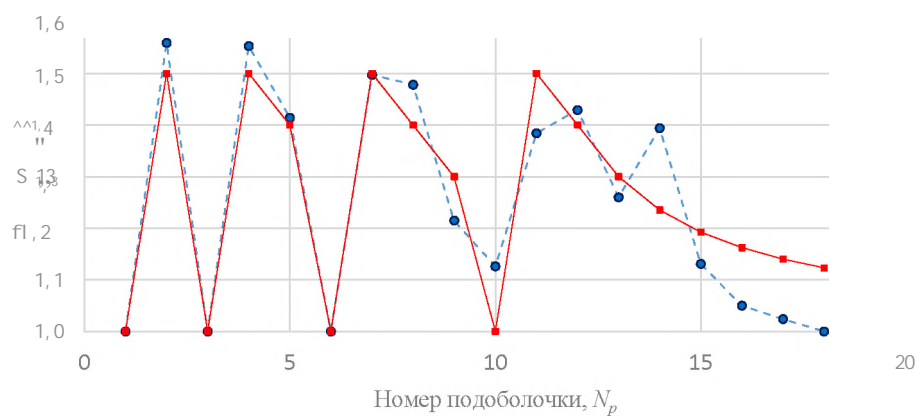
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 $4^{1/2}$. K

(5)

: 0 (), 1, 2, 3 . .


$$3 - \quad K_r \quad Np. \quad (5)$$

(5),

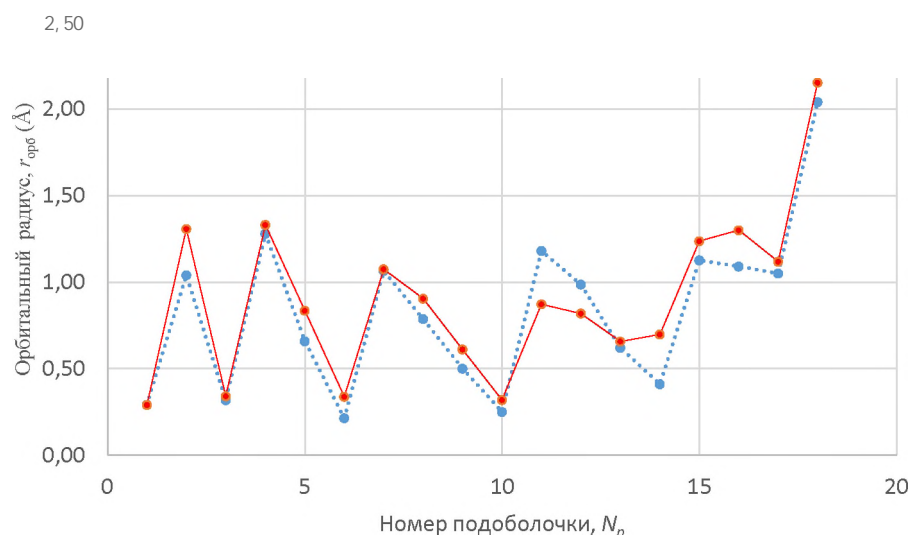
(1)

(4)

$$\hat{H} + \mathbf{l} \cdot \mathbf{Z} - (iV_p - 2/3) \quad (6)$$

(6)

4.



4 -

 $N_p: \bullet -$

[8], • -

(6)

(6)

$$=/(2)$$

$$K_r$$

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